

Performance Challenges for Simulation of Turbulent Flows in Complex Geometries

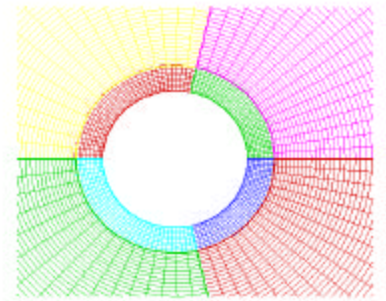
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Large-Eddy Simulations (LES)

- Solve unsteady Navier-Stokes and energy equation by resolving all scales of turbulence up to the inertial range *on the computational mesh* ($N \propto \text{Re}^2$)
 - turbulent length and time scales now decided explicitly by the mesh $\sim dx$.
 - Scales smaller than dx are not included and have to be modeled - subgrid stress modeling
 - Captures relevant turbulent physics with good fidelity - but **compute intensive**
 - Also **data intensive**

Alliance Funding

- Development and deployment of GenIDLEST
- General Incompressible Direct and Large-Eddy Simulations of Turbulence
 - Boundary conforming transformations
 - Multi-block structured grid
 - Unstructured block topology
 - x -direction boundary can interface with h - or z -direction boundary with arbitrary axes orientations
 - Non-matching block interfaces
 - Allows zonal embedding and flexibility in meshing complex geometries
 - Distributed/shared memory parallel computing technology



Current Applications

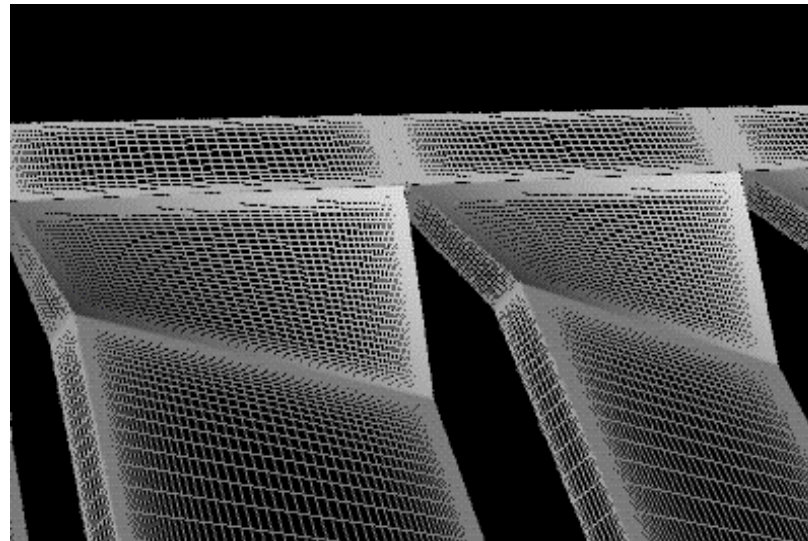
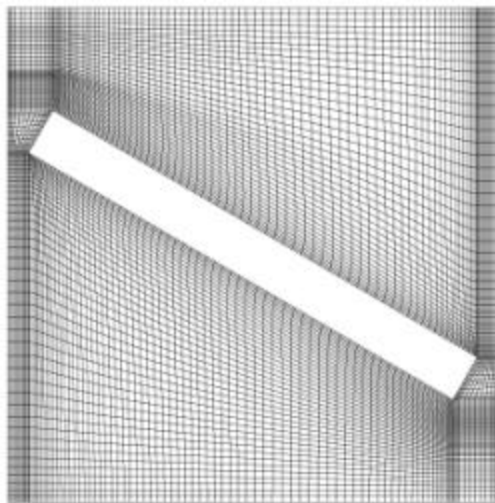
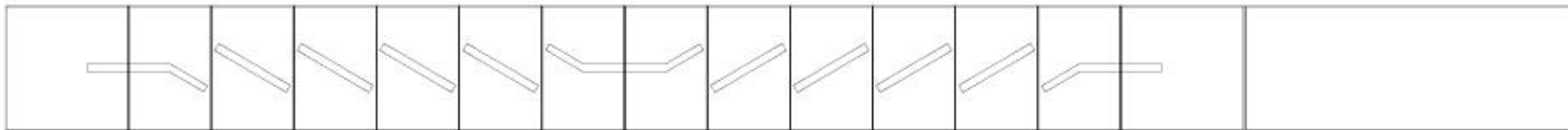
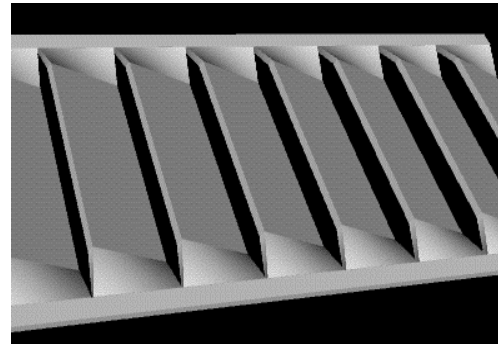
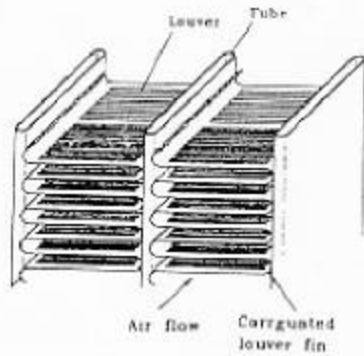
- Air-side heat transfer enhancement in compact heat exchangers
- Turbomachinery – internal/film cooling and combustors
- Process Equipment
- Microflows: lab-on-a-chip applications

Other Users:

Shell Oil

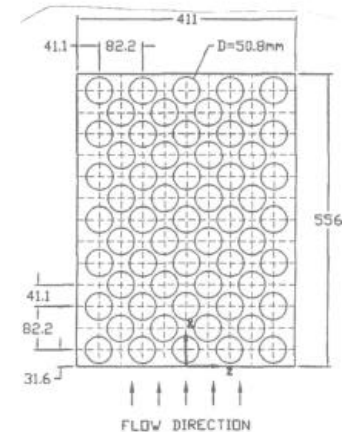
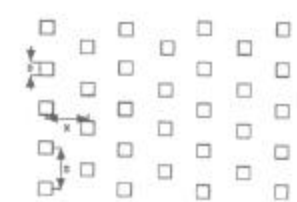
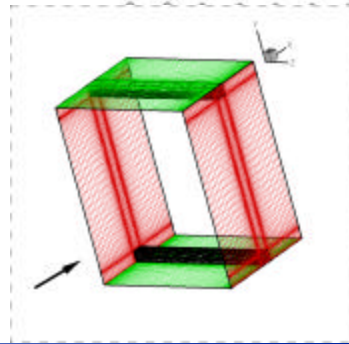
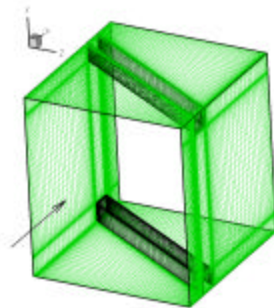
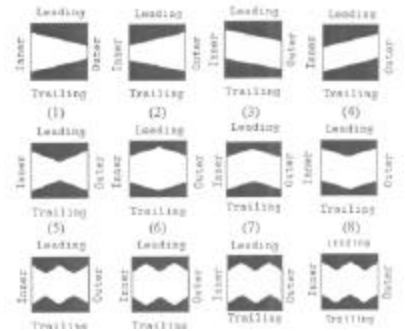
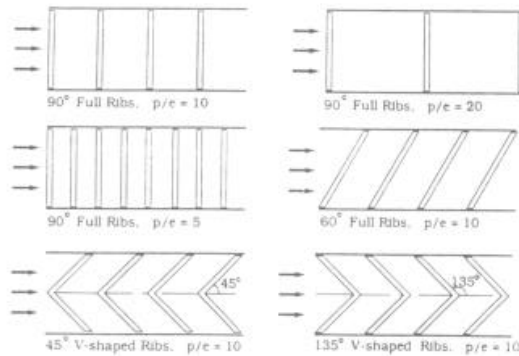
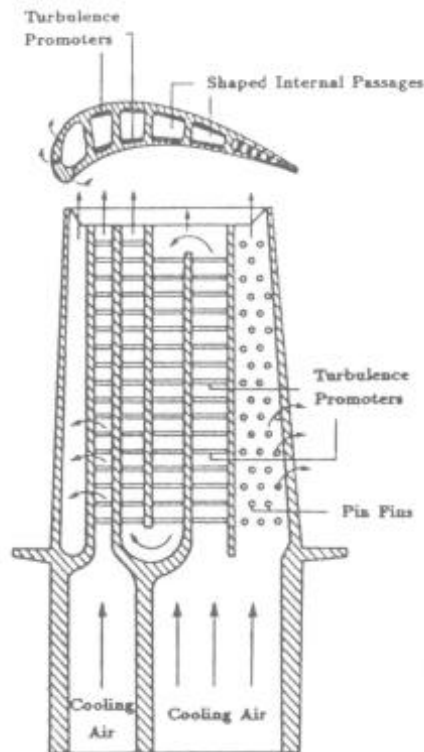
Virginia Active Combustion Control Group (VACCG)

Compact Heat Exchangers - Industry

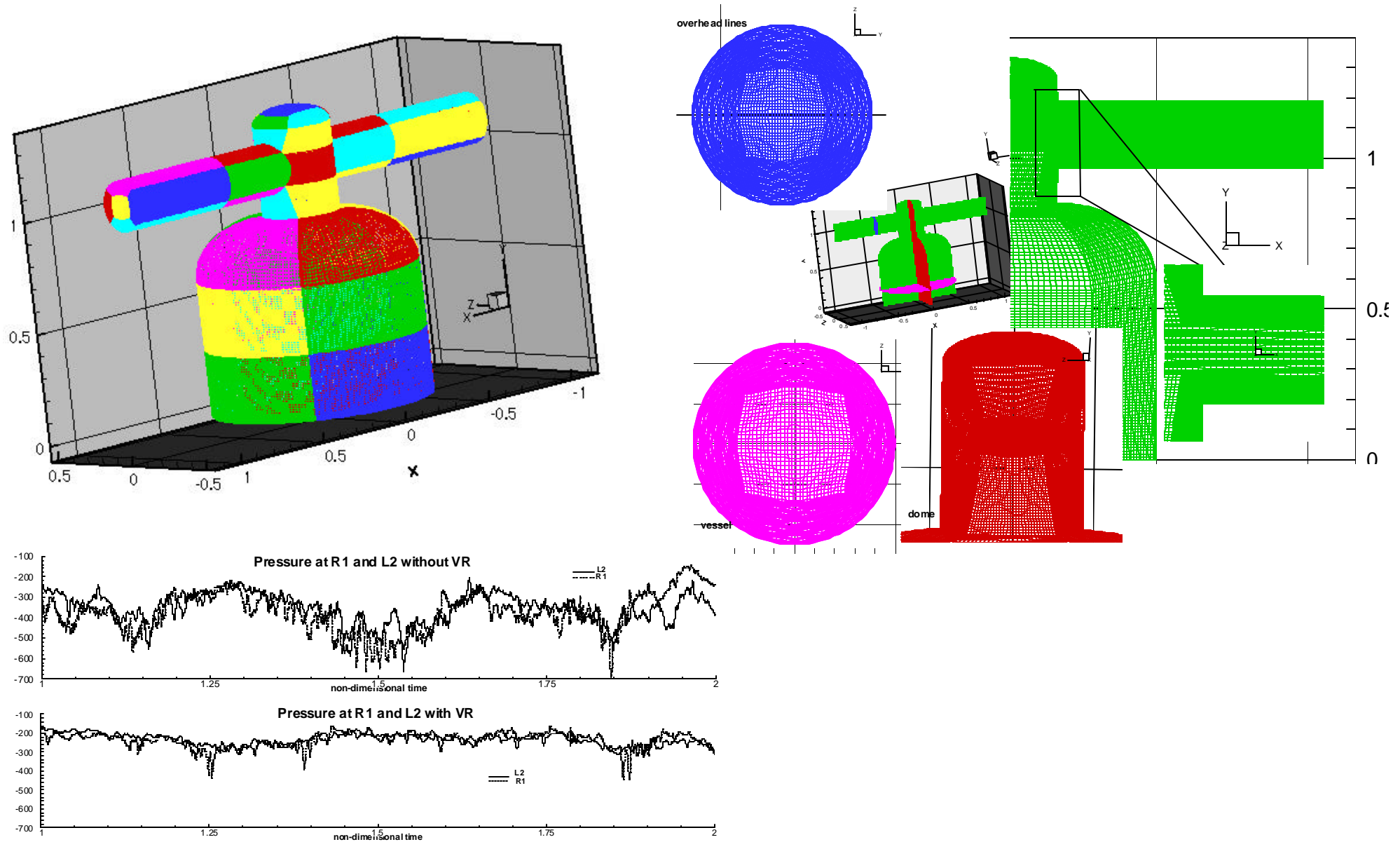


Internal Turbine Blade Cooling – DOE/industry

- **Flow is unsteady and turbulent, $Re \sim 20 - 50,000$.**
 - square, rectangular or trapezoidal channels
 - augmentation through ribs - roughness elements



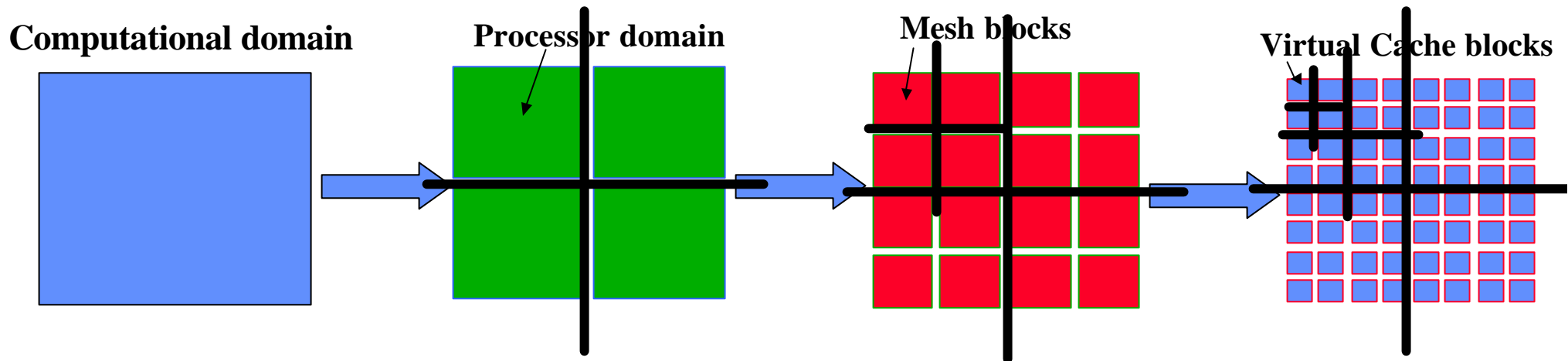
Flow Induced Vibrations in a Flasher Unit – Shell Oil



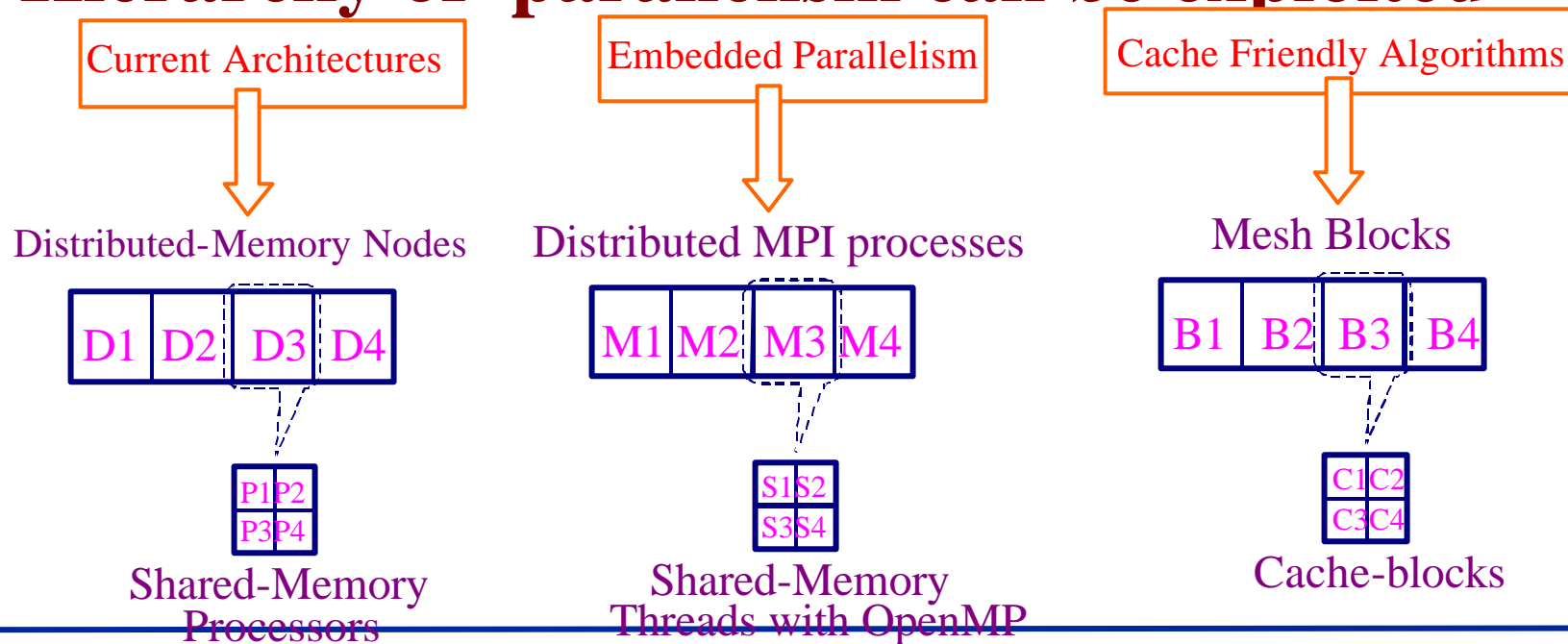
Dependent Technologies

- **Single processor performance – solution of linear systems and sparse-matrix vector operations**
- **Parallel computing paradigms (MPI, OpenMP)**
- **Parallel I/O, data (MPI-IO/HDF5)**
- **Distributed visualization and analysis (VisBench)**
- **GRID technologies: Globus, COG, PSE's.....**

GenIDLEST - Parallel Implementation



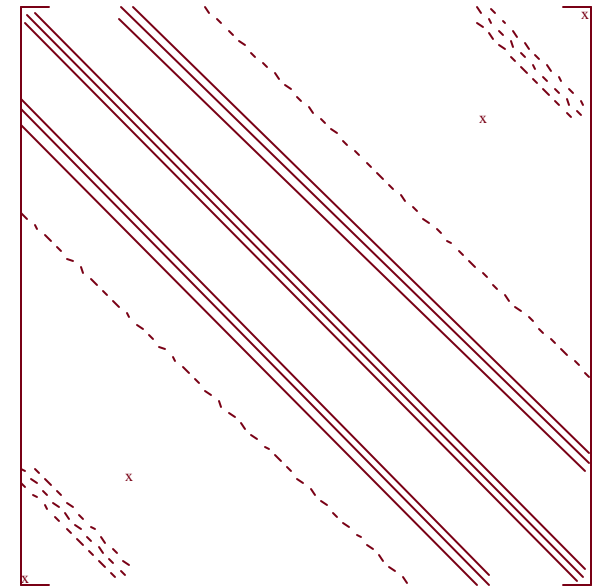
- Hierarchy of parallelism can be exploited**



Global System matrix

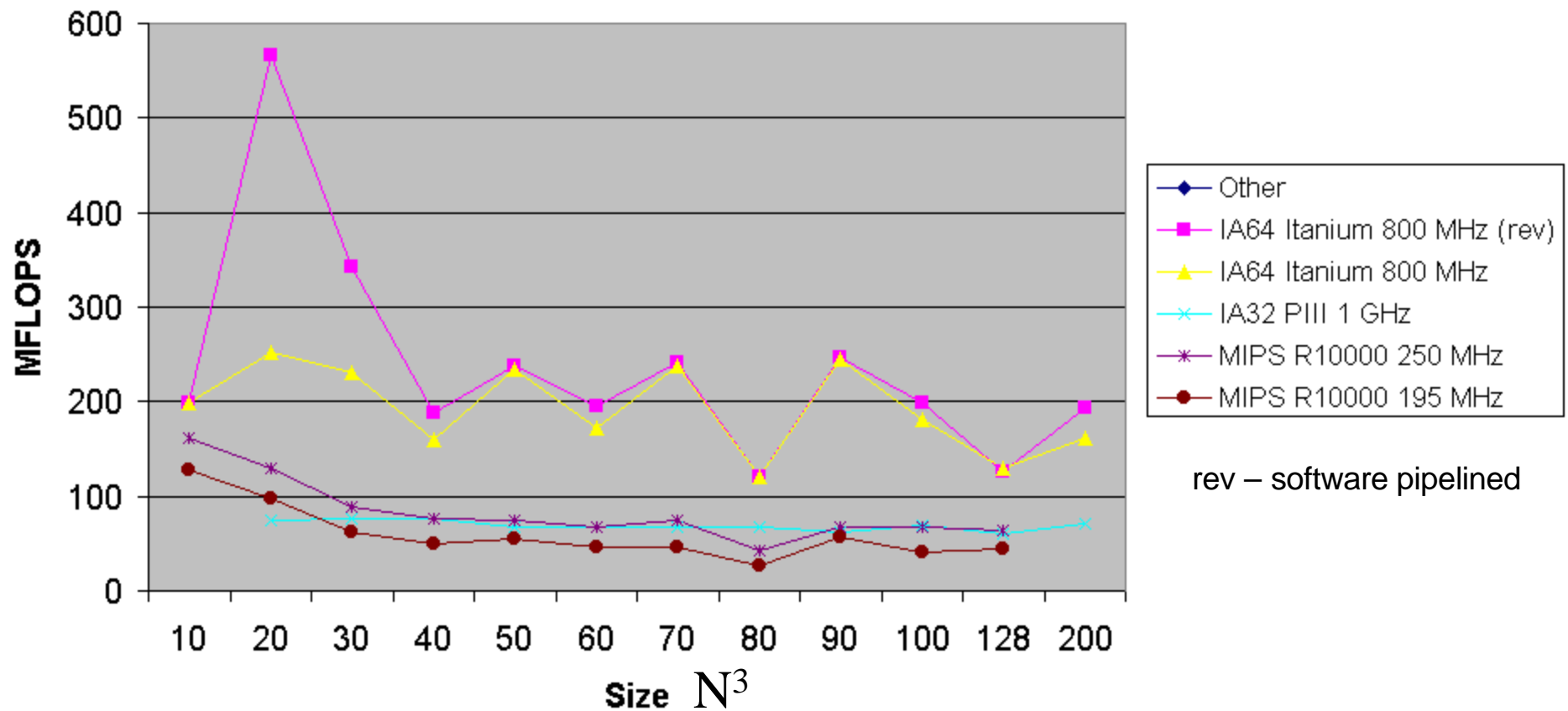
- Generated in semi-implicit treatment and pressure equation. 80-90% of computational work in complex geometries.
- **Sparse**
 - sparsity pattern depends on B.C.s.
 - Mostly non-symmetric-18 off-diagonal elements in 3-D
- Use CG for SPD systems, and BiCGSTAB, GMRES(m) for nonsymmetric.
- Preconditioners: Additive Schwarz Richardson or SSOR iterations applied to cache blocks.

2D system matrix,
— Non-periodic b.c.s
— Periodic b.c.s



Cross-Platform

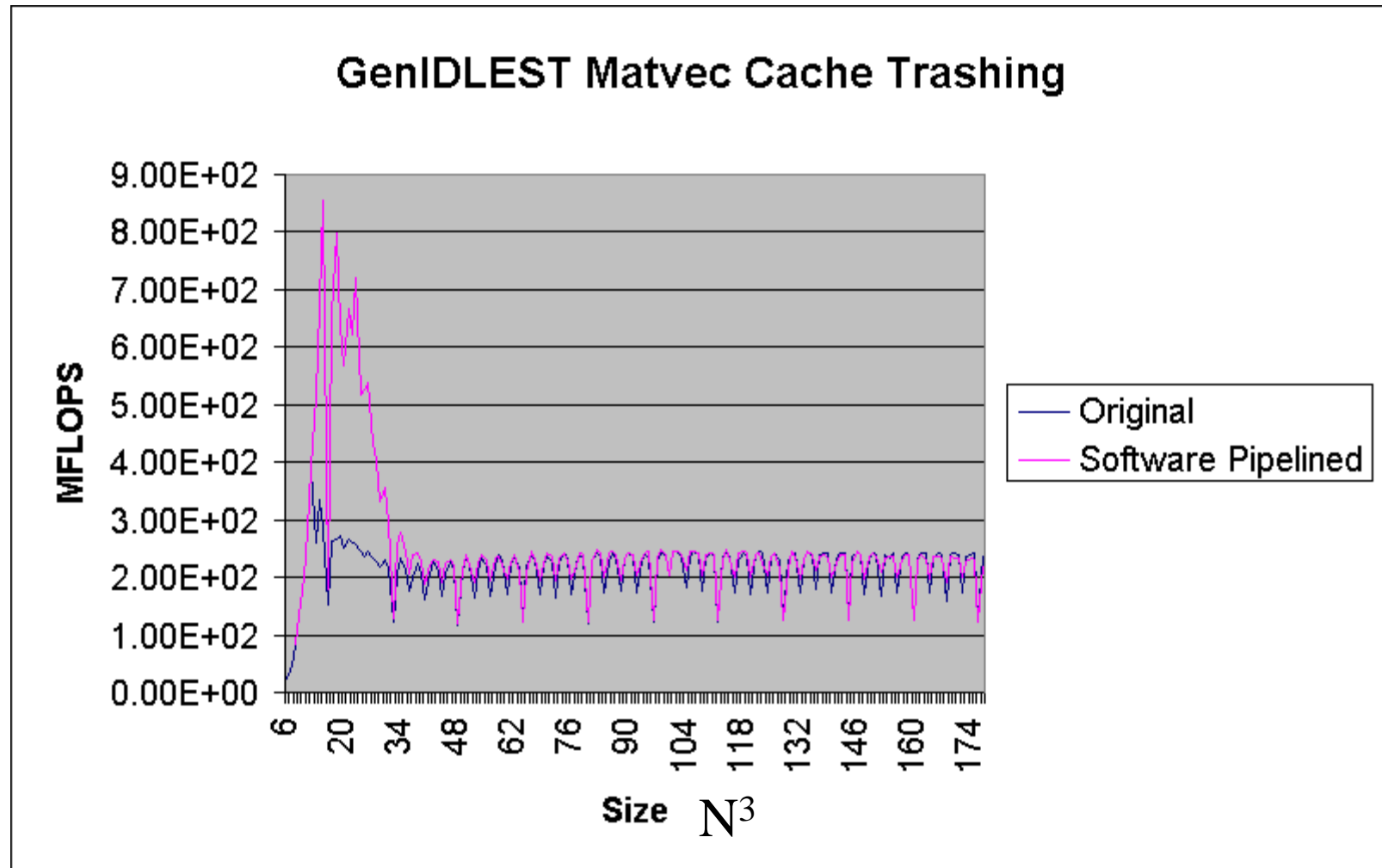
GenIDLEST Matrix-Vector Multiply Kernel (single processor)



rev – software pipelined

Rick Kufrin, NCSA Performance Engineering

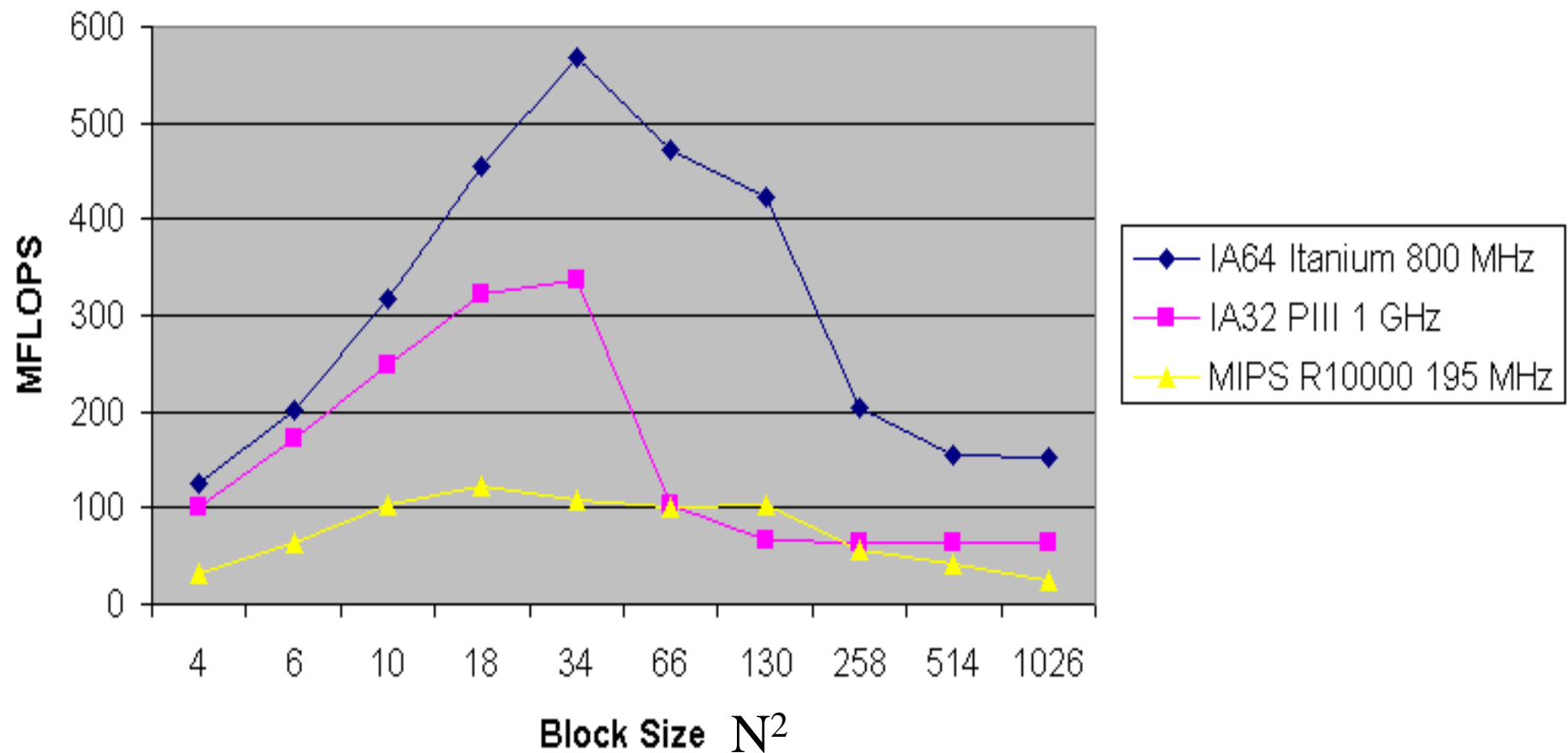
Itanium performance



Rick Kufrin, NCSA Performance Engineering

Linear Solver Performance

ASPCG Kernel Single-Processor



Rick Kufrin, NCSA performance engineering

Performance Challenges

- **Better Cache utilization**
 - Sparse matrix vector multiplies
 - Linear solvers
- **Load Balancing**
 - Block sizes, physics, processors – static.
- **General portable implementation of Fast Solvers based on 2-D and 3-D FFTs and linear solves for homogeneous problems.**